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SPIN DENSITY IN Cu_2O PLANE OF $YBa_2Cu_30_7$ PROBED BY Cu^{2+}NMR MEASUREMENTS

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ABSTRACT

The nuclear magnetic resonance (MMR) Spin lattice relaxation time (T_1^{-1}) are calculated for ^{63}Cu sites in $Yba_2Cu_30_7$. The calculations are based on the phenomenological model of Millis et.al. (1990) and the random phase approximation analysis of NMR by Bulut et. al. (1990).

The results are compared with experiments. The antiferomagnetic length is estimated to be 2.3 lattice constant at T = 100k and the total number of spins in the two dimensional plane is found to be temperature dependent. The findings make excitons mediated superconductivity conceivable [Isihara (1993)].

INTRODUCTION

The Cu spin-lattice relaxation rate is enhanced by antiferomagnetic spin correlations. The discussion of the relaxation rate depends on the model one chooses to describe the doped holes.

The two-band model allows the holes occupying the 2p orbital on oxygen to have degrees of freedom independent of the d holes on copper. The doped holes are mobile and carry spin.

In the single band model holes having primarily 2p character hybridize strongly with copper d holes of opposite spin forming a local singlet. The oxygen is symmetrically located between neighboring coppers so hyperfine fields from antiparallel spins on the neighboring coppers will cancel at the oxygen site.

According to Monien et.al. (1991), there is enough evidence to establish that a single band model of the planar spin excitations is sufficient to explain the nuclear spin relaxation rate in copper

The paper organized as follows: In section II, the hyperfine Hamiltonian, MMR and nuclear relaxation times are discussed. In section III, the parameter $\varepsilon(o)/a$ is determined. In section IV, the experimental results are used to determine the temperature dependence of the number of spins in the two dimensional plane. The conclusions are presented in section V.

II The Hamiltonian of the hyperfine interaction copper oxide superconductors is determined by the polarization of the s-electrons of the corresponding atoms due to the hybridization with holes in the 3d $(x^2 - y^2)$ states at planar copper sites. The hyperfine interaction for copper consists two parts: the first, is an anisotropic interaction due to spin-orbital coupling of 3d holes and dipole interaction at the same copper site. The second is a transferred hyperfine interaction due to polarization of 4s copper shells by 3d spins at neighboring copper sites. The hyperfine Hamiltonian for the planar copper atom is,

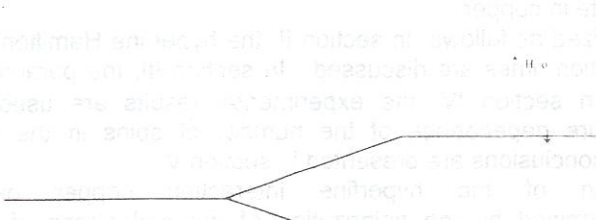
$$H_{hf} = \sum_{i,\alpha} A_{\alpha\alpha} I^{\alpha} S_i^{\alpha} + \sum_{\langle ij\rangle\alpha} B I^{\alpha} S_j^{\alpha}$$

Where $A_{\alpha\alpha}$ is the copper direct hyperfine tensor two component $A_{\perp}$ and $A_{\|}$;B is the transferred hyperfine coupling of the copper nucleus; S_i and S_j are the electron spins at the copper sites. They interact antiferromagnetically with a finite temperature dependent correlation length. I_j^{α} is the $\alpha-\text{th}$ component of the nuclear spin at site i and <ij> is the sum over the nearest neighbors j.

NUCLEAR MAGNETIC RESONANCE

Nuclear magnetic resonance is one of the principal spectroscopic tools use to study molecular structure. An atomic nucleus has a magnetic dipole moment μ, which may be expressed as $\mu = g_n \mu_{Bn} I$ where μ_{B_n} is the nuclear magneton g_n is the nuclear g-factor which varies from one nucleus to another. I is the spin quantum number, its allowed values are 0, ½, etc. When I = 0, then $\mu_n = 0$, and the nucleus evinces no magnetic response when I>0, the nucleus exhibits magnetic response. The nucleus of most interest in NMR is the one for which I = ½. This nucleus may be seen as a rotating spherical charge with the magnetic moment pointing in the direction of the axis of rotation. Those nuclei for which I > ½ in addition to their dipole moments they also have quadruple and even higher moments.

When an external field Ho is applied to the sample, the energy of the nucleus is split into (2I) sub levels. For I = ½, the multiplicity factor is 2, and hence the nuclear level splits into two sub-levels



The lower level corresponds to the nucleus moment pointing along the field Ho. The energy difference between the two levels is $\Delta E=2\mu nHo$ The system of nuclei is in resonance with an electromagnetic signal of frequency ν when the condition $h\nu = \Delta E$ is satisfied. That is $\upsilon = \frac{2\mu_n}{h}$ Ho, provided that the magnetic field of the lower level may absorb a photon from the signal and make a transition to the higher level.

The usefulness of NMR is based on the observation that the field felt by a nucleus inside the sample is not precisely equal to the external field Ho. This field is changed by a small field due to the environment in which the nucleus resides, and it is by measuring this additional field that we obtain information about the environment. The nucleus acts as our probe for investigating the internal structure through its monitoring of the environmental field. The nucleus in solid state is surrounded by electrons as well as by nearby atoms and molecules, which form its natural environment

NUCLEAR RELAXATION

When a static field is applied to a system of dipoles (nuclei with I = ½), these dipoles eventually turn around and align themselves predominantly with the field. In doing so they lose some magnetic energy. This loss of dipole energy must be dissipated, which can happen only if the dipoles are coupled to their environment in some manner.

Broadly speaking the vibration of the lattice atoms surrounding the dipole creates an oscillating field, which act on the dipole and absorbs energy from it. Thus the higher the temperature, the greater the interaction, and the shorter the time it takes to absorb magnetic energy from the dipoles. Usually its time $\tau_1 \approx 1/T$; a typical value at nitrogen temperature $\tau_1 = 10^{-6}_{S}$ The time is known as the longitudinal time or as the spin lattice relaxation time.

The dipole has also a transverse motion. Starting with its initial value, the vector $\vec{m}$ approaches its final equilibrium value $\vec{m}=0$ after a time equal to τ_2 this time is called the transverse relaxation time or spin – spin relaxation time. This time is usually very short and it is independent of temperature. It does however depend on the concentration of the magnetic atoms.

III PARAMETER CALCULATION

Anisotropic calculations are important in the determinations of the parameters associated with the nuclear spin-lattice relaxation rate relation. The anisotropy calculation that have been made are: $^{63}W_\perp$, $^{63}W_{11}$ and $^{17}W_\perp$. $^{63}W_\perp$ is the fundamental rate for $^{63}Cu(2)$ for a field applied in the a-b plane. $^{63}W_{11}$ is the fundamental rate for $^{63}Cu(2)$ for a field applied parallel to the c axis. ^{17}W is the isotropic fundamental rate for $^{17}O(2)$ nucleus.

According to Millis et. al (1991), $^{63}W_{11}/^{63}W_{\perp} = 3.50 \pm 0.40$. The paper by Imai et.al (1993) reported that $^{63}W_{11}/^{17}W = 19 \pm 2$. The above two reported measurements were done on the YBa_2CuO_7 system at a temperature of 100K. Making use of the above measurements in addition to the relationship due to Millis et.al. (1990),

$$\left[\frac{\varepsilon(T)}{a}\right]^2 = \left[\frac{\varepsilon(o)}{a}\right]^2 \frac{T_x}{TyT_x} \quad (1)$$

where $\varepsilon(T)$ is the correlation length, a is lattice constant, T is temperature $T > T_c$ where T_c is the superconducting transition temperature, the value of $[\varepsilon(o)/a]^2$ is calculated to be 9.52.

In the calculation for $\left[\frac{\varepsilon(o)}{a}\right]^2$, one used T_x = 120K and $\beta = \pi^2$ in conformity with the work of Millis et al. (1990).

IV Cu RELAXATION RATE

Millis et.al (1990) showed that $^{63}W_{11} = a + b\,T$, where $a = 666.7s^{-1}$ and $b = 1.9K^{-1}s^{-1}$. This expression is based on the analysis of the experimental measurements of $^{63}W_{11}$. However, the analytical expression for the same quantity is [Aiyohuyin, 1998]

$$^{63}W_{11} = \frac{\pi \aleph_0 k_B T A^2}{\mu_\beta^2 N \hbar^2 \Gamma}\left[0.157\beta(\varepsilon/a)^2 - 0.112\beta/n(\varepsilon/a) - 0.06213 + 0.410\right] \quad (2)$$

Where χ_o is the temperature dependent static susceptibility, Γ is the temperature dependent spin – fluctuation energy of the quasi particle,

$\beta = \left[\frac{a}{\varepsilon(o)}\right]^4$ and measures the relative strength of the antiferromagnetic paramagnon contribution to static susceptibility.

Following Monien et.al (1991), the following equations were used in the calculations

$$\frac{\chi_o(T)}{\mu_B} = [1.01 + 0.041(T/100)] \text{ states/ ev } Cu^{2+} \quad (3)$$

$$\Gamma(T) = [0.5 - T/2500] \text{ ev } Cu^{2+} \quad (4)$$

The hyperfine value used in the calculation is $A_{zz} = -1.519 \times 10^{-6}$ ev

The table below shows the result of the calculations

T(K)	$\left[\frac{\varepsilon(T)}{a}\right]^2$	$\left[\frac{\varepsilon(T)}{a}\right]$	$\hbar\Gamma(T)x1.6x10^{-19}$ J	$\chi(T)/\mu_\beta^2\,x(1.6x10^{-19})^{-1}$ $\frac{state}{J}$	$W_{11}(T)\ s^{-1}$	N
200	3.57	1.89	0.42	1.830	1046.7	3.79
250	3.09	1.76	0.40	2.035	1141.7	4.18
300	2.72	1.65	0.38	2.240	1236.7	4.69
350	2.43	1.56	0.36	2.445	1331.7	5.20
400	2.20	1.48	0.34	2.650	1426.7	5.75
450	2.50	1.41	0.32	2.855	1521.7	6.30
500	1.84	1.36	0.30	3.060	1616.7	6.91

The physical meaning or interpretation of N is given by Chakravarty and Orbach (1990) as the number of spins in the two dimensional plane of Cu_2O.

V CONCLUSION

The temperature dependence of the number of spins in 2 dimensional Cu_20 plane indicates that at the temperature considered a Bose – Einstein condensation of the paraexcitons has taken place. The excitons in Cu_20 interact probably with each other repulsively. Due to the low effective mass, a high critical temperature is expected [Akira Isihara (1993)]. It is probable that exciton mediate high temperature superconductivity just as phonons do for low-temperature superconductivity.

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